From Equality to Equivalence in Chemistry: Valence, Structure, and the Homotopy of Molecular Identity

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For centuries, the equality sign “=” has been a cornerstone of chemistry. It balances equations, equates reactants and products, and anchors the symbolic representation of molecular formulas. Yet equality is also a blunt instrument, one that collapses distinctions between entities that are clearly not identical but which nevertheless behave in structurally equivalent ways. Sodium and potassium are not equal atoms, but they are equivalent with respect to their valence shells; methane and ammonium ion are not equal molecules, but they share the same tetrahedral geometry under VSEPR theory. Resonance structures, isoelectronic species, and homologous groups all testify to the fact that chemistry, like mathematics, operates primarily “up to equivalence.” By importing insights from Category Theory and Homotopy Type Theory—especially the univalence perspective that equivalence can serve as identity—we can recast chemical sameness in a more faithful light. Molecules, atoms, and phases need not be forced into rigid equality, but can instead be recognized as members of structured equivalence classes. This shift clarifies chemical reasoning, aligns with existing practice, and offers a new conceptual foundation for the philosophy and pedagogy of chemistry.

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1. Introduction: Chemistry and the Limits of Equality

The equality sign "=" has long served as one of the most recognizable symbols in chemistry. From the earliest alchemical recipes to modern chemical equations, it is the mark of balance and sameness. In stoichiometry, "=" signals that the number of atoms on one side of an equation matches those on the other; in formula writing, it asserts that hydrogen and oxygen combine to yield water; in thermodynamics, it ties state variables together in precise mathematical form. Equality, in this sense, has been indispensable: it allows chemists to calculate yields, to conserve mass, and to express the fundamental symmetries of matter. Without the simplicity of "=," chemical notation would lack its elegance and its calculational power.

And yet, equality is also a blunt instrument. Chemistry constantly confronts us with cases where two entities are not literally the same but act in structurally equivalent ways. Sodium and potassium are different atoms, yet their outer valence shells make them chemically interchangeable in many contexts. Methane and the ammonium ion differ in composition and charge, but both adopt a tetrahedral geometry under VSEPR theory. Benzene is not equal to any one of its Lewis structures, but is equivalent across them through resonance. In each case, what matters to chemistry is not rigid identity but functional or structural equivalence.

This recognition opens the door to a deeper framework. Just as Homotopy Type Theory in mathematics reframes identity as equivalence, chemistry too can benefit from a language that honors structural correspondences without collapsing them into literal equality. By reinterpreting chemical sameness through the lens of Category Theory and HoTT, we can see atoms, molecules, and reactions not as rigid entities bound by "=," but as participants in equivalence classes of structure and behavior. This perspective provides not only a faithful reflection of chemical practice but also a conceptual bridge between mathematics and chemistry, suggesting that "$\simeq$" may one day stand where "=" has long reigned.

2. Atomic Equivalence: The Periodic Table

At the atomic level, chemistry makes immediately clear that strict equality is too rigid to capture chemical reality. Sodium is not potassium. Their nuclei differ in proton number, neutron count, and mass. Their physical properties—melting point, density, spectral lines—are distinct. By any literal measure, Na ≠ K. Yet, when placed in the context of chemical bonding, sodium and potassium are functionally interchangeable. Both occupy Group 1 of the periodic table, both have a single electron in their outermost shell, and both readily donate that electron to form +1 cations. In chemical reactions, sodium and potassium often play identical roles, substituting for one another with only modest differences in reactivity.

The genius of Mendeleev's periodic table was precisely this recognition: the table organizes elements not by absolute identity, but by equivalence of valence-shell structure. Groups in the table are equivalence classes—sets of elements that, despite differences in nuclear detail, share structural features that dictate chemical behavior. This is why chlorine, bromine, and iodine are grouped as halogens, why calcium and strontium fall together as alkaline earths, and why neon and argon are both noble gases. The periodic system does not flatten differences into equality, but arranges elements into structural families defined by equivalence.

From the perspective of Homotopy Type Theory, this maps naturally onto the concept of identity types. In HoTT, two terms are not declared identical by fiat, but can be considered "the same" if there exists a path—an equivalence—connecting them. Sodium and potassium are distinct terms in the universe of atoms, but there exists a structural equivalence path between them: their shared valence shell. That path allows chemists to treat them as "the same" in many contexts, just as univalence allows equivalent types to be treated as identical in mathematics.

Thus, the periodic table itself can be read as a living example of $\simeq$, not =. It encodes not literal identities of elements, but structured equivalences that predict behavior across families. Where classical equality would collapse sodium and

potassium into sameness or exclude any relation at all, equivalence preserves their difference while highlighting their shared capacity for coherence.

3. Valence Shell and VSEPR Equivalence

If the periodic table reveals equivalence at the level of atoms, then Valence Shell Electron Pair Repulsion (VSEPR) theory reveals it at the level of molecules. VSEPR classifies molecular shapes according to the repulsion between electron pairs in the valence shell of the central atom. What emerges from this model are recurring spatial patterns—linear, trigonal planar, tetrahedral, trigonal bipyramidal, octahedral—that recur across many different molecules.

Take the tetrahedral geometry. Methane (CH_4), the ammonium ion (NH_4^+), and silane (SiH_4) differ in elemental composition, total electron count, and physical properties. They are not equal molecules—$CH_4 \neq NH_4^+ \neq SiH_4$. Yet, each arranges its bonding pairs in identical tetrahedral fashion. In chemical reasoning, this structural equivalence matters more than literal identity: once a molecule is classified as tetrahedral, we know its bond angles, its approximate symmetry, and even something about its chemical reactivity.

VSEPR theory, then, is a taxonomy of equivalence classes. Each class is defined not by rigid equality but by shared spatial arrangement. Molecules assigned to the same class are structurally equivalent with respect to geometry, even if they differ in every other respect. The geometry itself is an invariant—preserved across substitutions of central atom and ligands, so long as the valence-shell electron configuration matches.

In Homotopy Type Theory, such reasoning finds a natural parallel. Different molecules correspond to different terms, but their shared VSEPR class functions like an identity type: it provides a structured context in which these molecules can be considered “the same.” Their equivalence is not literal identity but a path through geometry—a homotopy that reveals coherence across difference.

Thus, VSEPR demonstrates how chemistry already operates “up to equivalence.” It recognizes that molecules are not defined solely by their atoms, but by the

structural role of their valence shells. This perspective is exactly what HoTT formalizes: sameness is a matter of structured correspondence, not blunt equality.

4. Isoelectronic and Isostructural Equivalence

Equivalence in chemistry is not limited to atomic valence or gross molecular geometry. A subtler but equally powerful lens is provided by isoelectronicity and isostructurality—concepts that classify species by shared electron counts and orbital structures rather than by chemical formula.

Two species are called isoelectronic if they possess the same number of electrons and a similar arrangement of orbitals. For example, carbon monoxide (CO) and nitrogen (N_2) both contain 14 total electrons. When analyzed through molecular orbital (MO) theory, each exhibits the same sequence of bonding and antibonding orbitals, with identical bond orders and comparable bond lengths. They are not equal molecules—one is a heteronuclear diatomic, the other homonuclear—yet their electronic structures are effectively interchangeable. In many contexts, chemists treat $CO \simeq N_2$, recognizing that their bonding behavior arises from equivalence at the orbital level.

A parallel principle applies to isostructural molecules, those that share an overall spatial geometry despite different atomic compositions. Boron trifluoride (BF_3) and the carbonate ion (CO_3^{2-}) illustrate this. BF_3 is a neutral trigonal planar molecule with delocalized electron deficiency, while CO_3^{2-} is an anion with resonance-delocalized π bonds. They differ in charge, composition, and bonding detail, but both adopt trigonal planar symmetry with 120° bond angles. In structural reasoning, chemists regard $BF_3 \simeq CO_3^{2-}$ with respect to geometry, using one as a proxy for predicting the shape of the other.

These examples demonstrate that chemistry repeatedly invokes equivalence classes defined by electron count or orbital arrangement, much as Category Theory defines equivalence by structure-preserving transformations. CO and N_2 are distinct terms, but their molecular orbital diagrams establish a path of

equivalence. BF_3 and CO_3^{2-} are distinct formulas, yet they converge under the same geometrical type.

The analogy to Homotopy Type Theory is direct. In HoTT, objects are not considered equal in isolation but equivalent within a higher structure that mediates identity. Isoelectronic and isostructural classifications do the same for molecules: they define identity not as literal equality but as equivalence witnessed by shared electron configurations or geometries. Chemistry thus embodies the HoTT principle that sameness is structural, contextual, and relational.

5. Resonance and Higher Path Equivalence

One of the most striking demonstrations of equivalence in chemistry arises in the treatment of resonance structures. Consider benzene (C_6H_6). In classical Lewis notation, benzene can be drawn in at least two distinct ways: one with alternating single and double bonds starting at one carbon, and another with the double bonds shifted around the ring. Neither of these drawings is *equal* to benzene. In fact, no single Lewis structure captures the true nature of its bonding. The actual molecule possesses a delocalized π system in which six electrons are spread evenly across the ring, producing equivalent bond lengths between all carbon–carbon pairs.

Chemists resolve this mismatch not by discarding Lewis structures, but by invoking resonance: benzene is understood as a resonance hybrid, an entity equivalent to *all* of its contributing structures, though not equal to any single one of them. Each structure is a witness to part of its identity; the whole is the equivalence class of all resonance forms together.

This logic mirrors the higher path structure of Homotopy Type Theory. In HoTT, two terms may be related by multiple distinct identifications (paths). These identifications are not collapsed into one; rather, they themselves can be related by higher paths—homotopies between homotopies. Benzene is analogous: there are multiple “paths” (resonance structures) that witness its identity, and the true

molecule is not reducible to any one witness but to the coherent system of all. The equivalence of benzene's resonance structures is a higher-dimensional sameness that transcends equality.

More generally, delocalized π systems—such as those found in conjugated polyenes, aromatic heterocycles, or carbonate anions—express this same principle. They are not adequately described by a single bonding pattern, but by an equivalence class of structures linked by resonance. In pedagogical terms, chemistry has long practiced a higher-dimensional understanding of identity: coherence emerges not from any one formula, but from the structured interplay of many.

In this way, resonance offers a perfect analogue to HoTT's higher paths. Both reveal that identity is not a single blunt assertion but a hierarchy of correspondences. Benzene is not equal to any of its drawings, just as a type is not equal to a single proof of identity. Instead, its truth is borne out by the web of equivalences that bind multiple witnesses into a coherent whole.

6. Chirality and Conditional Equivalence

Chirality provides one of the richest cases where equivalence in chemistry is conditional—it depends on which structural features are chosen for preservation. Two molecules are chiral enantiomers if they are non-superimposable mirror images of one another, such as L-glucose and D-glucose. From the perspective of connectivity, bonding, and molecular formula, these two species are structurally equivalent: each has the same atoms, the same covalent framework, and the same stereogenic centers arranged in opposite configurations. If the criterion of equivalence is merely bond connectivity, then L-glucose $\simeq$ D-glucose.

Yet functionally, the distinction matters. Biological systems often discriminate sharply between enantiomers. Human enzymes and receptors, themselves chiral, will metabolize D-glucose efficiently but treat L-glucose as an inert or ineffective sugar. Thus, if the equivalence relation we preserve is *chemical bonding structure*, the molecules are equivalent. If the equivalence relation we preserve is *biological*

activity, they are not. Equality cannot capture this subtlety, but equivalence, as a relative and context-dependent relation, can.

In Homotopy Type Theory, this maps directly onto the idea that equivalence is relative to the universe or context in which identity is considered. Two objects may be equivalent in one universe of discourse but distinct in another. For instance, two types may be equivalent up to homotopy in one categorical framework, yet fail to be equivalent when additional constraints are imposed. L-glucose and D-glucose illustrate precisely this: they are structurally equivalent in the abstract space of stereochemistry but distinct in the biological universe of enzymatic recognition.

This example shows how equivalence is not absolute but defined relative to what structures we preserve. Chirality demonstrates that equivalence can be geometrical, functional, or contextual. Equality collapses all nuance into a rigid verdict, but equivalence allows chemistry—and HoTT—to encode *what matters* in a given domain. In this sense, chirality is not a failure of equivalence, but a refinement: it shows that sameness is not universal but mediated by the structures we choose to privilege.

7. Phase and Polymorphic Equivalence

Another domain where chemistry demonstrates the inadequacy of rigid equality is in phases of matter. Consider water. Ice, liquid water, and vapor are not equal: they differ in density, intermolecular arrangement, and physical properties. A crystal of ice cannot be mistaken for a drop of liquid, nor a drop for steam. Yet at the molecular level, they are all H_2O. The identity of the molecule is preserved across phase transitions, which serve as paths of transformation between states. Under equality, we are forced into awkward statements—ice ≠ water ≠ vapor. Under equivalence, we can say: ice ≃ liquid ≃ vapor, all equivalent under the structural identity of H_2O.

A similar pattern is found in polymorphism, where a single element forms multiple crystalline structures. Carbon is the clearest example. Diamond, graphite, and

graphene differ radically in hardness, conductivity, and dimensionality. Diamond has sp^3 hybridized carbon in a tetrahedral lattice; graphite has sp^2 hybridization in layered sheets; graphene isolates one such sheet in two dimensions. By equality, they are wholly distinct substances. By equivalence, they are recognized as coherent variants: C atoms with four valence electrons, arranged under different hybridization schemes. The structural equivalence is mediated by valence, not literal sameness.

These examples provide a striking analogy to higher homotopy in HoTT. In homotopy theory, points in a space may be connected by paths, and paths themselves may be connected by higher homotopies. Likewise, ice can be transformed continuously into liquid, and liquid into vapor; graphite can be transformed into diamond under pressure. These are not equalities but paths of equivalence—coherence across distinct states. At a higher level, all these phases or polymorphs are equivalent within the type "H_2O" or "elemental carbon," linked by transformations that preserve molecular or atomic identity.

Thus, phase and polymorphic transitions illustrate equivalence as continuity across transformation. Equality would treat each state as isolated, while equivalence recognizes them as connected members of a higher structure. Chemistry, once again, anticipates the HoTT perspective: sameness is not a rigid fact but a network of transformations that bind distinct states into a coherent whole.

8. Philosophy and Pedagogy of Equivalence in Chemistry

Chemistry has always been, at its heart, a structuralist science. Its explanatory power lies not in asserting that two entities are literally identical, but in recognizing patterns and equivalences across apparent differences. The classification of functional groups is a prime example: alcohols, aldehydes, ketones, carboxylic acids, and amines are not equal molecules, yet each class shares a structural fragment that governs characteristic reactivity. A homologous series extends this further: methane, ethane, propane, and butane differ in chain

length, but all are equivalent under the repeating $–CH_2–$ unit. The periodic table itself is a grand act of structuralism, arranging elements into equivalence classes defined by valence behavior rather than rigid identity.

Seen in this light, chemistry has always operated more in terms of $\simeq$ than =. Equality reduces substances to blunt sameness, ignoring distinctions that matter. Equivalence, by contrast, allows chemists to preserve structural differences while still identifying coherence across families of compounds. The equivalence of functional groups, homologous series, isoelectronic species, resonance forms, and phases captures the living practice of the field far more faithfully than strict equality.

This recognition has important pedagogical implications. Chemistry is often taught with heavy reliance on the equality sign: balanced equations, empirical formulas, stoichiometric ratios. While these are indispensable tools, they risk misleading students into thinking of chemical identity as rigid sameness. A more faithful approach is to teach chemistry explicitly "up to equivalence." From the very beginning, students can be shown that sodium and potassium are equivalent in valence behavior, that methane and ammonium ion are equivalent in geometry, and that benzene's multiple Lewis structures are equivalent witnesses of its identity. Such framing aligns chemical pedagogy with the actual reasoning chemists use in practice, and it harmonizes chemistry with the broader intellectual shift in mathematics from equality to equivalence.

Philosophically, this transition reframes the ontology of chemistry. Substances are no longer isolated "things" defined by equality, but participants in networks of equivalence: groups, families, and structures connected by transformation. This mirrors the insight of Homotopy Type Theory—that identity is mediated by structure, not given as a primitive. By teaching chemistry in these terms, we not only clarify its internal logic but also bridge it conceptually to mathematics, physics, and even philosophy. In doing so, we prepare the next generation to see science as a universe of equivalences, rather than a flat landscape of equalities.

9. Speculative Vision: Chemistry Through HoTT

If Homotopy Type Theory has transformed mathematics by shifting the foundation from equality to equivalence, then chemistry may be poised for a similar reframing. Instead of treating atoms, molecules, and reactions as rigidly distinct entities, we can recast chemical ontology as a hierarchy of equivalence classes. Atoms belong to periodic families defined by valence-shell equivalence; molecules belong to structural classes defined by VSEPR geometries, functional groups, or isoelectronic counts; resonance forms and polymorphs represent higher-path equivalences within those classes. Chemistry already works this way in practice—HoTT simply offers a formal language to express it.

The implications are far-reaching. In chemical informatics, databases could be organized not by exact molecular identity alone, but by equivalence classes that capture structural or functional similarity. Searches could operate on "$\simeq$" rather than "=," retrieving families of compounds unified by reactivity rather than formula. In AI-driven molecular design, models trained on equivalence classes could generalize far more effectively, generating novel molecules that preserve structural roles rather than merely replicating known entities. In quantum chemistry, where wavefunctions describe states up to phase and symmetry, HoTT-like reasoning could offer new tools for classifying solutions by equivalence rather than literal equality.

This vision points toward a future in which $\simeq$ underlies chemical knowledge just as it now underlies modern mathematics. Chemistry would no longer be forced into the rigid framework of equality, but would instead be understood as a landscape of transformations, symmetries, and higher correspondences. Molecules, atoms, and phases would be studied as members of structured families, linked by equivalences that preserve what matters while respecting difference.

Such a foundation could unify chemistry with broader scientific and philosophical frameworks. Just as mathematics after Voevodsky now regards equivalence as the true measure of sameness, chemistry may come to see equivalence as its most faithful ontology. In this speculative but promising direction, we glimpse a science

that is not only more coherent but also more creative—able to generate new knowledge by navigating the universe of equivalences that defines matter itself.

10. Conclusion

The equality sign “=” has been indispensable to the development of chemistry. It allowed equations to be balanced, reactions to be quantified, and formulas to be written with clarity and precision. Without it, the calculational rigor of stoichiometry, thermodynamics, and kinetics would not have been possible. Equality gave chemistry its backbone, just as it did for mathematics.

Yet, equality is too blunt to capture the full richness of chemical reality. Sodium is not potassium, though they are equivalent in valence behavior. Methane is not ammonium ion, though both are tetrahedral. Benzene is not any single Lewis structure, but a resonance hybrid across many. Chirality, polymorphism, and isoelectronicity all demonstrate that chemistry is filled with cases where rigid identity fails, and where equivalence better reflects structural and functional sameness. Chemistry has always operated informally in this way; equivalence is how chemists actually reason, even if they still write “=.”

Homotopy Type Theory makes this implicit logic explicit in mathematics, declaring equivalence to be the true foundation of identity. Chemistry may be ready for a similar transformation. By adopting equivalence as the lens through which atoms, molecules, and reactions are understood, the discipline can align its philosophy with its practice, and its pedagogy with its deepest insights. Just as HoTT has recast the foundations of mathematics, equivalence may reshape the foundations of chemistry—revealing that sameness is not a rigid fact, but a structured coherence across difference.

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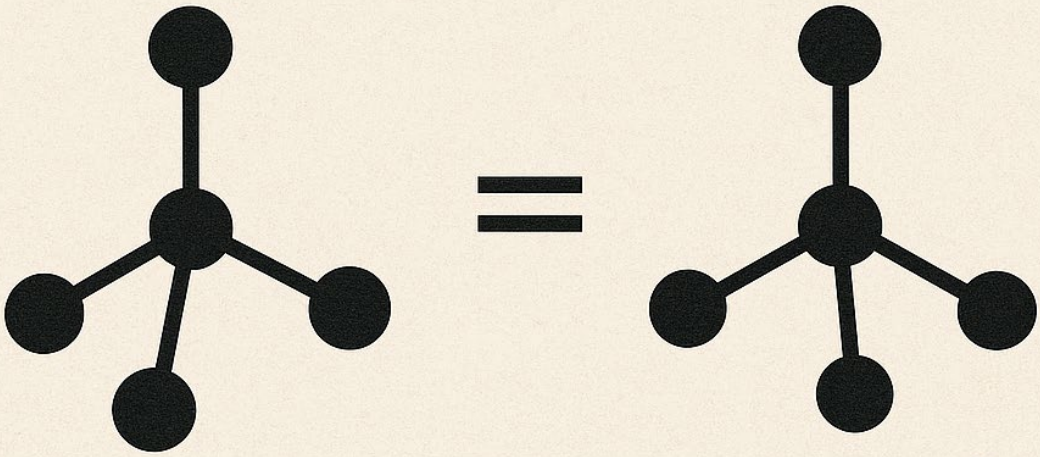

NH_4^+

Structural Equivalence